WE CLAIM:

1. A method for displaying a three dimensional representation of a structure of a protein comprising:

taking machine readable data comprising structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2;

computing a three dimensional representation of a structure based on the structure coordinates; and

displaying the three dimensional representation.

2. A method according to claim 1, wherein the root mean square deviation is less than or equal to 0.65.

3. A method according to claim 1, wherein the root mean square deviation is less than or equal to 0.49.

4. A method according to claim 1, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

5. A method according to claim 1, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

6. A method for displaying a three dimensional representation of a structure of a protein comprising:

displaying a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than 0.98 when the coordinates used to compute the surface contour are compared to the structure coordinates of Figure 3, if the comparison is based on alpha-carbon atoms in both the protein being modeled and the amino acid residues specified in Table 2 and the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the amino acid residues specified in Table 2.

7. A method according to claim 6, wherein the root mean square deviation is less than or equal to 0.65.

8. A method according to claim 6, wherein the root mean square deviation is less than or equal to 0.49.

9. A method according to claim 6, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

10. A method according to claim 6, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

11. A computational method comprising:

taking machine readable data comprising structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2;

computing phases based on the structural coordinates;

computing an electron density map based on the computed phases; and

determining a three-dimensional crystal structure based on the computed electron density map.

12. A method according to claim 11, wherein the root mean square deviation is less than or equal to 0.65.

13. A method according to claim 11, wherein the root mean square deviation is less than or equal to 0.49.

14. A method according to claim 11, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

15. A method according to claim 11, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

16. A computational method comprising:

taking an X-ray diffraction pattern of a crystal of the target protein; and

computing a three-dimensional electron density map from the X-ray diffraction pattern by molecular replacement, wherein structure coordinates used as a molecular replacement model comprise structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2.

17. A method according to claim 16, wherein the method further comprises determining a three-dimensional crystal structure based upon the computed three-dimensional electron density map.



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18. A method according to claim 16, wherein the root mean square deviation is less than or equal to 0.65.

19. A method according to claim 16, wherein the root mean square deviation is less than or equal to 0.49.

20. A method according to claim 16, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

21. A method according to claim 16, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

22. A method for evaluating a potential of an entity to associate with a protein comprising:

creating a computer model of a protein structure using structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2;

performing a fitting operation between the entity and the computer model; and

analyzing results of the fitting operation to quantify an association between the entity and the model.

23. A method according to claim 22, wherein the root mean square deviation is less than or equal to 0.65.

24. A method according to claim 22, wherein the root mean square deviation is less than or equal to 0.49.

25. A method according to claim 22, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

26. A method according to claim 22, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

27. A method for evaluating a potential of an entity to associate with a protein comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than 0.98 when the coordinates used to compute the surface contour are compared to the structure coordinates of Figure 3 if the comparison is based on alpha-carbon atoms in both the protein being modeled and the amino acid residues specified in Table 2 and the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the amino acid residues specified in Table 2;

evaluating a potential of an entity to associate with the surface contour by performing a fitting operation between the entity and the surface contour; and

analyzing results of the fitting operation to quantify an association between the entity and the computer model.

28. A method according to claim 27, wherein the root mean square deviation is less than or equal to 0.65.

29. A method according to claim 27, wherein the root mean square deviation is less than or equal to 0.49.

30. A method according to claim 27, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.



Express Mailing No. EL978337886US

31. A method according to claim 27, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

32. A method for identifying potential agonists or antagonists comprising:

generating a three-dimensional structure of a protein using structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2;

employing the three-dimensional structure to design or select a potential agonist or antagonist; and

contacting the agonist or antagonist with a protein having at least 55% identity with SEQ. ID No. 1.

33. A method according to claim 32, wherein the root mean square deviation is less than or equal to 0.65.

34. A method according to claim 32, wherein the root mean square deviation is less than or equal to 0.49.

35. A method according to claim 32, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

36. A method according to claim 32, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

37. A method for identifying potential agonists or antagonists comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than 0.98 when the coordinates used to compute the surface contour are compared to the structure coordinates of Figure 3 if the comparison is based on alpha-carbon atoms in both the protein being modeled and the amino acid residues specified in Table 2 and the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the amino acid residues specified in Table 2;

employing the three-dimensional structure to design or select a potential agonist or antagonist; and

contacting the agonist or antagonist with a protein having at least 55% identity with SEQ. ID No. 1.

38. A method according to claim 37, wherein the root mean square deviation is less than or equal to 0.65.

39. A method according to claim 37, wherein the root mean square deviation is less than or equal to 0.49.

40. A method according to claim 37, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

41. A method according to claim 37, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

42. A method for evaluating the ability of an entity to associate with a protein, the method comprising:

constructing a computer model defined by structure coordinates that comprise structure coordinates that have a root mean square deviation equal to or less than 0.98 when compared to

the structure coordinates of Figure 3, the root mean square deviation being calculated such that the alpha-carbon atom positions of each set of structure coordinates are superimposed and the root mean square deviation is based only on those amino acid residues in the structure coordinates that are also present in the portion of the protein specified in Table 2;

selecting an entity to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the entity, (ii) selecting an entity from a small molecule database, (iii) *de novo* ligand design of the entity, and (iv) modifying a known ligand for MvaS, or a portion thereof;

performing a fitting program operation between computer models of the entity to be evaluated and the binding pocket in order to provide an energy-minimized configuration of the entity in the binding pocket; and

evaluating the results of the fitting operation to quantify the association between the entity and the binding pocket model in order to evaluate the ability of the entity to associate with the said binding pocket.

43. A method according to claim 42, wherein the root mean square deviation is less than or equal to 0.65.

44. A method according to claim 42, wherein the root mean square deviation is less than or equal to 0.49.

45. A method according to claim 42, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

46. A method according to claim 42, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.

47. A method for evaluating the ability of an entity to associate with a protein, the method comprising:

computing a computer model for a protein binding pocket, at least a portion of the computer model having a surface contour that has a root mean square deviation equal to or less than 0.98 when the coordinates used to compute the surface contour are compared to the structure coordinates of Figure 3 if the comparison is based on alpha-carbon atoms in both the protein being modeled and the amino acid residues specified in Table 2 and the root mean square deviation is calculated based only on those amino acid residues present in both the protein being modeled and the amino acid residues specified in Table 2;

selecting an entity to be evaluated by a method selected from the group consisting of (i) assembling molecular fragments into the entity, (ii) selecting an entity from a small molecule database, (iii) *de novo* ligand design of the entity, and (iv) modifying a known ligand for MvaS, or a portion thereof;

performing a fitting program operation between computer models of the entity to be evaluated and the binding pocket in order to provide an energy-minimized configuration of the entity in the binding pocket; and

evaluating the results of the fitting operation to quantify the association between the entity and the binding pocket model in order to evaluate the ability of the entity to associate with the said binding pocket.

48. A method according to claim 47, wherein the root mean square deviation is less than or equal to 0.65.

49. A method according to claim 47, wherein the root mean square deviation is less than or equal to 0.49.

50. A method according to claim 47, wherein the root mean square deviation comparison is also based on main-chain atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.98.

51. A method according to claim 47, wherein the root mean square deviation comparison is also based on non-hydrogen atoms positions of the amino acid residues and the root mean square deviation is equal to or less than 0.89.